



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 02:12 PM UTC

PDB ID : 1TVK / pdb_00001tvk
Title : The binding mode of epothilone A on α,β -tubulin by electron crystallography
Authors : Nettles, J.H.; Li, H.; Cornett, B.; Krahn, J.M.; Snyder, J.P.; Downing, K.H.
Deposited on : 2004-06-29
Resolution : 2.89 Å (reported)
Based on initial model : 1JFF

This is a wwPDB EM Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

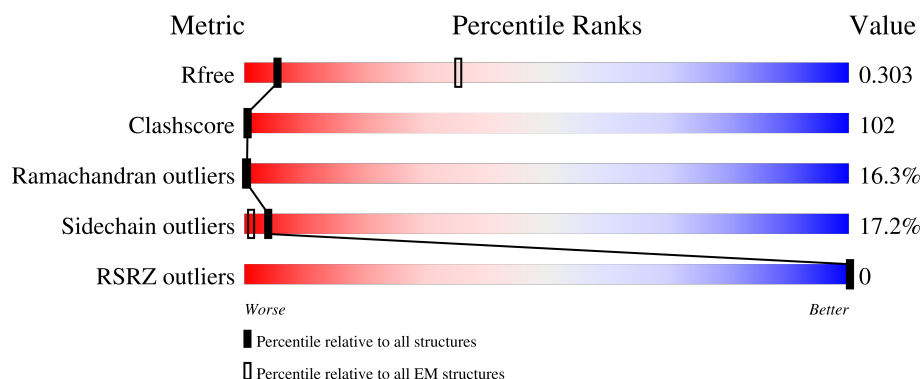
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

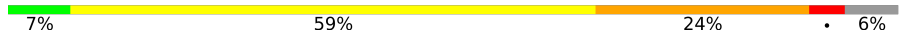
The reported resolution of this entry is 2.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
R_{free}	180332	208
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RSRZ outliers	180361	209

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	440	
2	B	427	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6672 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	412	Total	C	N	O	S	0	0
			3227	2043	551	613	20		

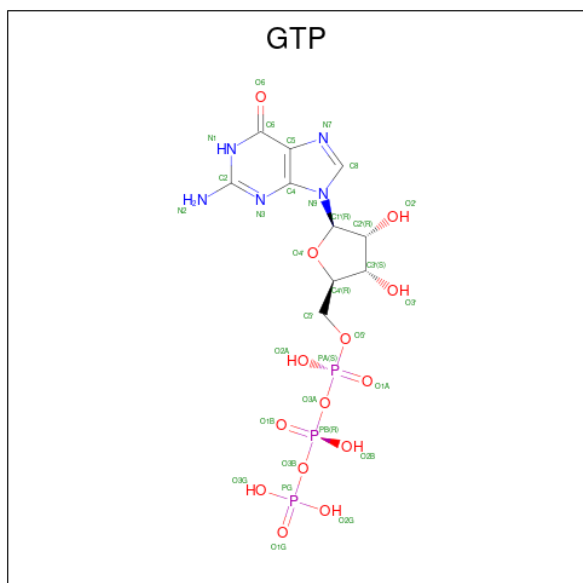
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

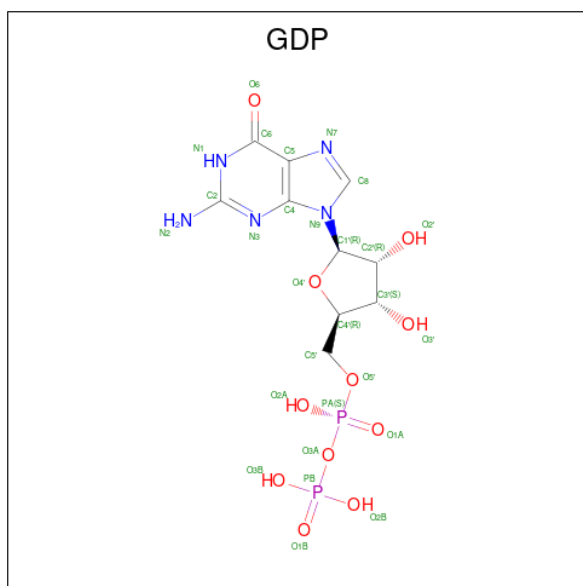
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	426	Total	C	N	O	S	0	0
			3351	2105	575	646	25		

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



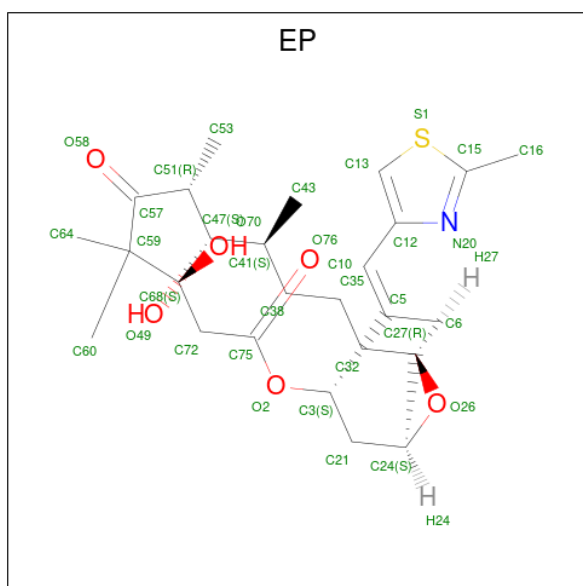
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 4 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
4	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 5 is EPOTHILONE A (CCD ID: EP) (formula: $C_{26}H_{39}NO_6S$).

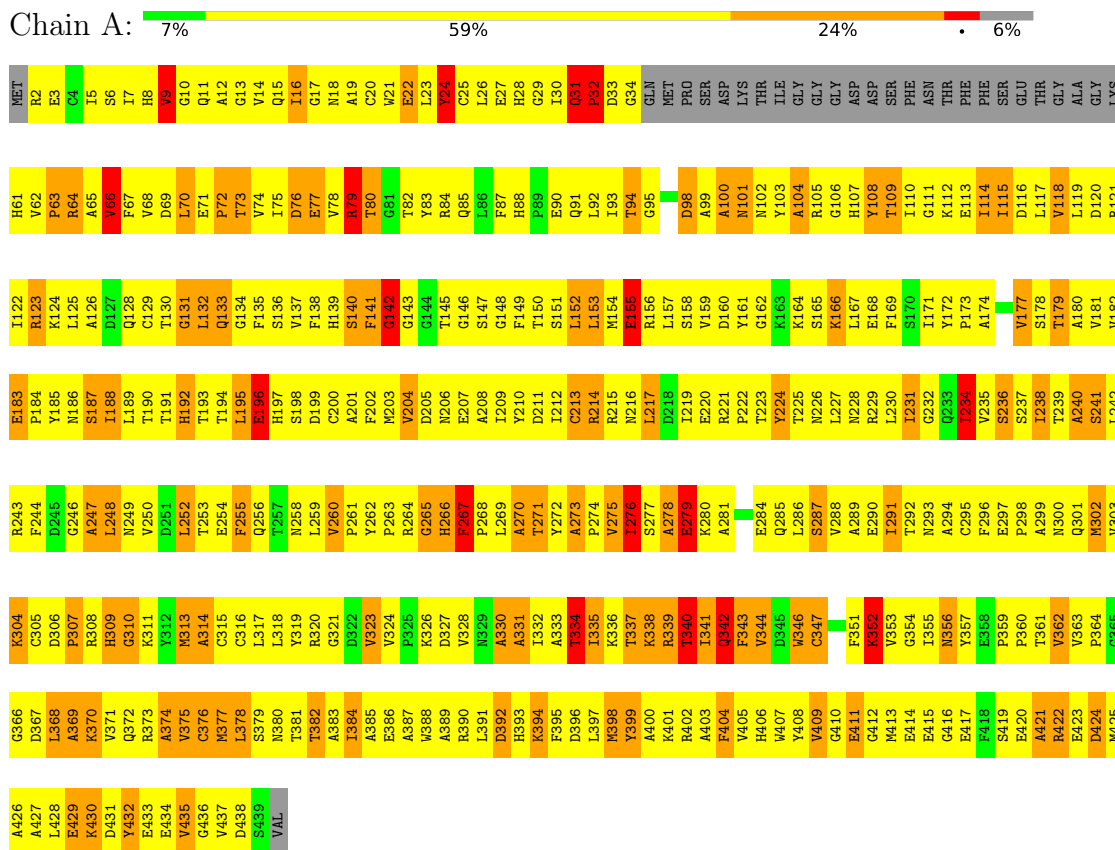


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
5	B	1	34	26	1	6	1	0

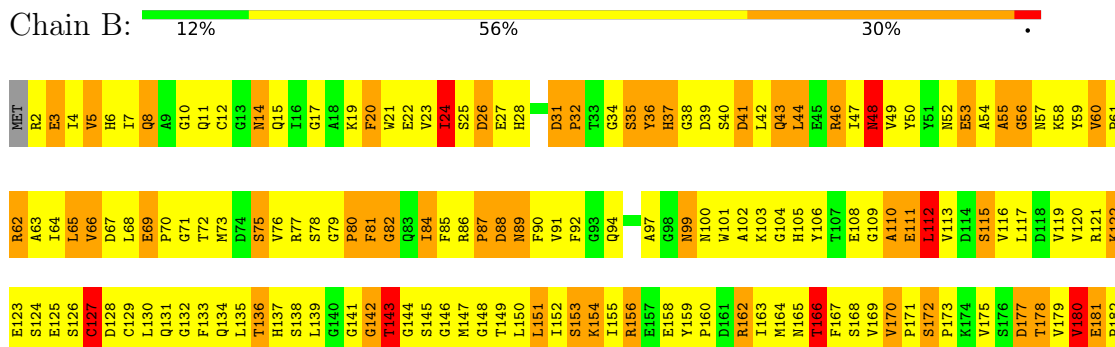
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin alpha chain



• Molecule 2: Tubulin beta chain



Q426 D427	T366 T367 T368 T369 T370 T371 T372 T373 T374 T375 T376 T377 T378 T379 T380 T381 T382 T383 T384 T385 T386 T387 T388 T389 T390 T391 T392 T393 T394 T395 T396 T397 T398 T399 T400 E401 G402 M403 D404 E405 M406 E407 F408 T409 E410 A411 E412 S413 M414 M415 M416 D417 L418 V419 S420 E421 Y422 Q423 Q424	P305 R306 H307 G308 R309 Y310 T311 T312 T313 V313 A314 A315 R318 G319 R320 M321 S322 M323 K324 E325 V326 D327 F328 Q329 M330 L331 V332 G333 Q334 N335 K336 N337 S338 S339 Y340 F341 V342 E343 D344 I345 P346 N347 N348 T349 K350 T351 A352 V353 C354 D355 I356 P357 F358 R359 G360 L361 Y362 K362 M363 S364 Q365	G244 Q245 L246 N247 A248 D249 L250 R251 K252 L253 A254 V255 N256 M257 V258 P259 F260 P261 R262 L263 H264 F265 F266 M267 P268 G269 F270 A271 T272 L273 T274 S275 R276 Q279 Q280 Y281 R282 A283 L284 T285 V286 P287 E288 L289 T290 Q291 Q292 M293 F294 D295 A296 K297 N298 M299 M300 A301 A302 G303 D304	Y183 N184 A185 T186 L187 S188 V189 H190 Q191 L192 A193 E194 N195 T196 D197 E198 T199 Y200 C201 L202 D203 N204 E205 A206 L207 Y208 D209 T210 C211 F212 R213 T214 L215 K216 L217 P220 T221 Y222 G223 D224 L225 M226 H227 L228 V229 S230 A231 T232 M233 S234 G235 V236 T237 T238 C239 L240 R241 F242 D243
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.20Å 93.50Å 90.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 2.89 90.00 – 2.89	Depositor EDS
% Data completeness (in resolution range)	67.0 (91.29-2.89) 63.7 (90.00-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 2.89Å)	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.333 , 0.321 0.314 , 0.303	Depositor DCC
R_{free} test set	967 reflections (3.36%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 3.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.096 for -h,-l,-k 0.070 for -h,l,k 0.118 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6672	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8280e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, EP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.60	0/3300	1.10	28/4482 (0.6%)
2	B	0.64	4/3426 (0.1%)	1.15	49/4642 (1.1%)
All	All	0.62	4/6726 (0.1%)	1.13	77/9124 (0.8%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	227	HIS	CE1-NE2	-6.68	1.25	1.32
2	B	227	HIS	CD2-NE2	6.06	1.44	1.37
2	B	227	HIS	CG-ND1	-5.83	1.31	1.38
2	B	282	ARG	NE-CZ	-5.07	1.27	1.33

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ILE	N-CA-C	-11.60	102.16	113.53
1	A	335	ILE	N-CA-C	-10.18	99.01	110.62
2	B	379	LYS	N-CA-C	-8.62	99.81	111.96
1	A	153	LEU	N-CA-C	-8.37	102.00	112.72
1	A	260	VAL	CA-C-N	7.95	127.50	119.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3227	0	3143	699	0
2	B	3351	0	3229	660	0
3	A	32	0	12	4	0
4	B	28	0	12	8	0
5	B	34	0	39	4	0
All	All	6672	0	6435	1332	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 102.

The worst 5 of 1332 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:HG2	1:A:15:GLN:HE21	1.04	1.12
2:B:172:SER:HB3	2:B:205:GLU:HG2	1.16	1.10
2:B:286:VAL:H	2:B:287:PRO:HD2	1.11	1.09
2:B:315:ALA:HB3	2:B:330:MET:HE1	1.35	1.08
1:A:229:ARG:HD3	1:A:363:VAL:HG21	1.33	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/440 (93%)	223 (55%)	113 (28%)	72 (18%)	0	0
2	B	424/427 (99%)	251 (59%)	109 (26%)	64 (15%)	0	0
All	All	832/867 (96%)	474 (57%)	222 (27%)	136 (16%)	0	0

5 of 136 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	VAL
1	A	72	PRO
1	A	73	THR
1	A	100	ALA
1	A	101	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/369 (94%)	290 (84%)	57 (16%)	2	8
2	B	367/368 (100%)	301 (82%)	66 (18%)	2	6
All	All	714/737 (97%)	591 (83%)	123 (17%)	4	7

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	3	GLU
2	B	329	GLN
2	B	69	GLU
2	B	307	HIS
2	B	381	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	264	HIS
2	B	384	GLN
2	B	298	ASN
2	B	347	ASN
2	B	416	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	EP	B	1001	-	36,36,36	1.89	7 (19%)	48,53,53	2.53	10 (20%)
3	GTP	A	9500	-	33,34,34	2.95	3 (9%)	50,54,54	0.69	1 (2%)
4	GDP	B	1500	-	29,30,30	1.95	1 (3%)	45,47,47	0.71	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EP	B	1001	-	-	15/50/55/55	1/3/3/3
3	GTP	A	9500	-	-	3/22/38/38	0/3/3/3
4	GDP	B	1500	-	-	2/16/32/32	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9500	GTP	PB-O3B	-10.54	1.48	1.59
4	B	1500	GDP	PA-O3A	-10.05	1.48	1.59
3	A	9500	GTP	PA-O3A	-9.43	1.49	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9500	GTP	PB-O3A	-8.68	1.50	1.59
5	B	1001	EP	C27-C24	7.52	1.60	1.46

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	EP	C27-O26-C24	12.29	69.53	60.67
5	B	1001	EP	O26-C27-C24	-6.38	55.15	59.66
5	B	1001	EP	O26-C24-C27	-6.13	55.32	59.66
5	B	1001	EP	C13-C12-N20	-2.86	108.82	113.56
5	B	1001	EP	O2-C75-C72	2.62	116.13	111.43

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1001	EP	C5-C10-C12-N20
5	B	1001	EP	C59-C68-C72-C75
5	B	1001	EP	O70-C68-C72-C75
5	B	1001	EP	C41-C47-C51-C53
5	B	1001	EP	O49-C47-C51-C57

All (1) ring outliers are listed below:

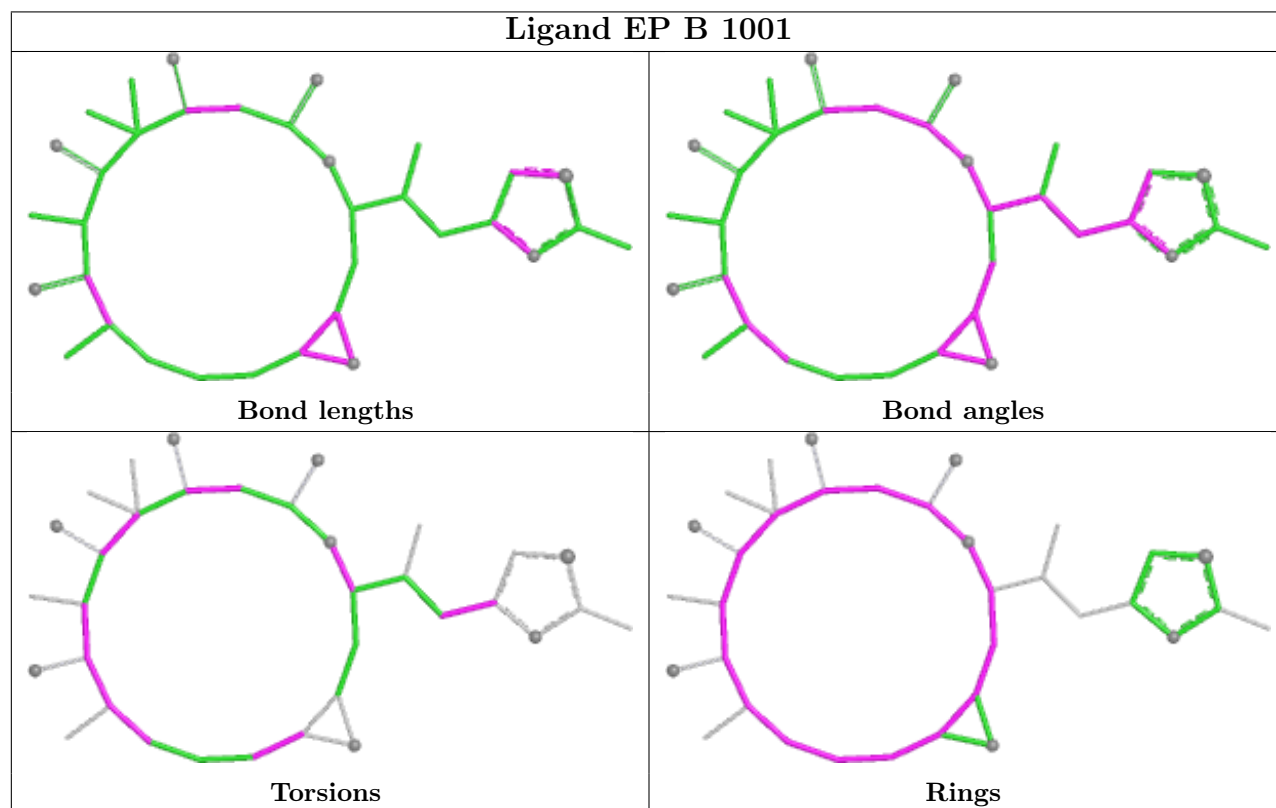
Mol	Chain	Res	Type	Atoms
5	B	1001	EP	C21-C24-C27-C3-C32-C35-C38-C41-C47-C51-C57-C59-C68-C72-C75-O2

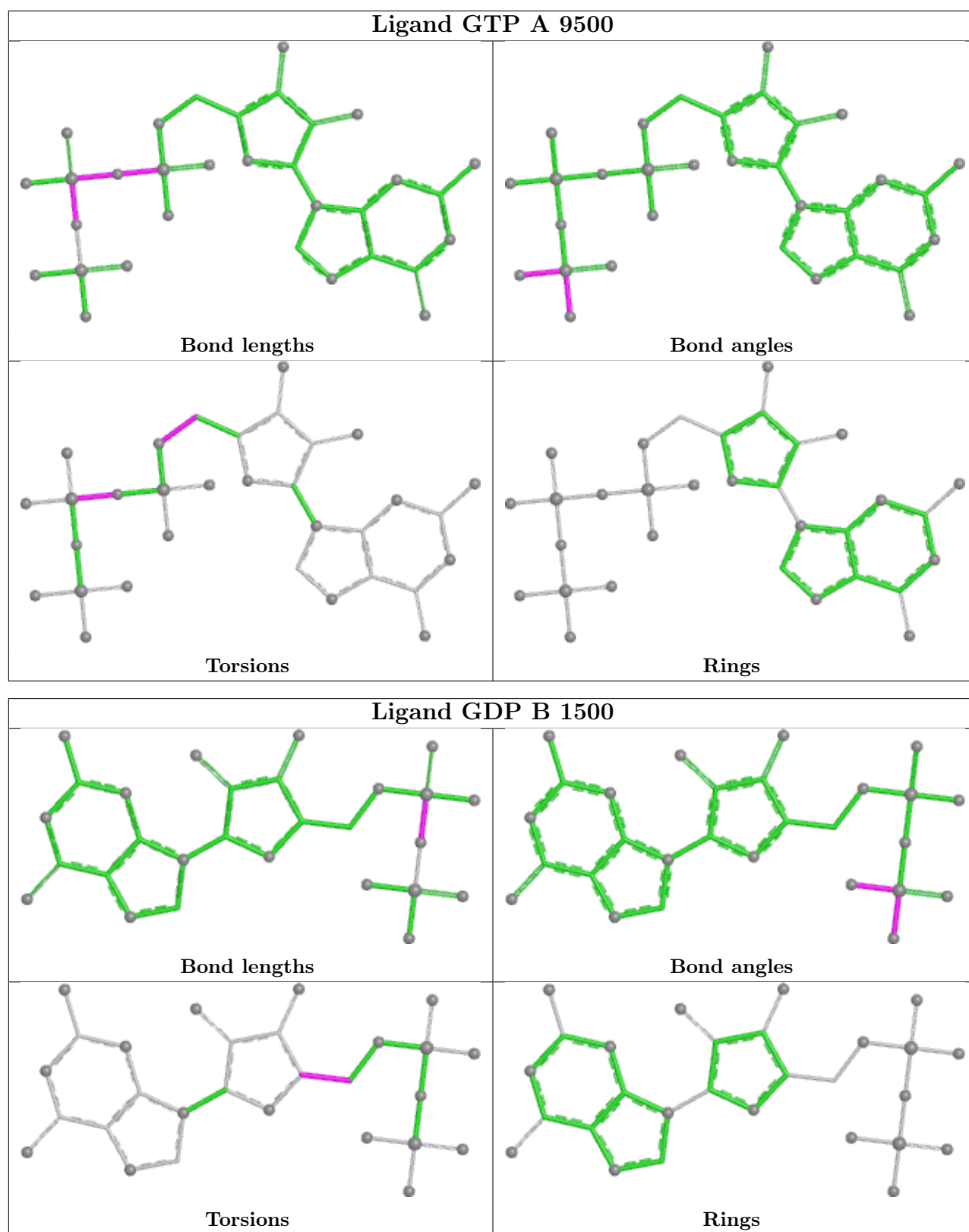
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	EP	4	0
3	A	9500	GTP	4	0
4	B	1500	GDP	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.